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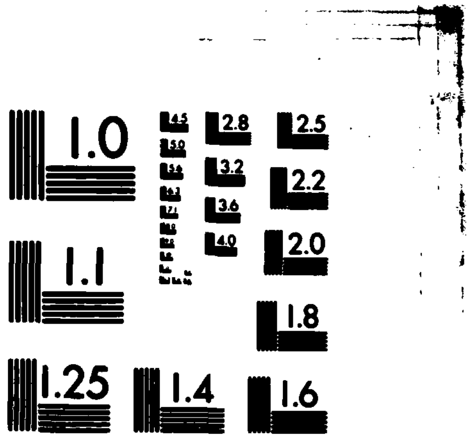
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TECHNICAL REPORT ARLCB-TR-84030

ELECTRICAL RESISTIVITY IN LOW RESISTIVITY AMORPHOUS ALLOYS

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OCTOBER 1984

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER
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The temperature dependence of the electrical resistivity in low resistivity ($\rho < 100$ μΩcm) amorphous alloys is analyzed in the framework of the diffraction model. The standard diffraction model yields results in qualitative agreement with the available data. However, a quantitative agreement with the data is observed if phonon ineffectiveness effects are included by means of the Pippard-Ziman constraint. A variety of results are presented for ranges of $2k_F/k_p$ and electron mean free paths.

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INTRODUCTION

The diffraction model (ref 1) provides the basis for quantitative studies of electrical transport in liquid and amorphous metals. Surprisingly good agreement with experimental data has been obtained. However, significant discrepancies between diffraction model predictions and the data are well known in high resistivity ($\rho > 100\ \mu\Omega\mathrm{cm}$) amorphous metals. Such discrepancies are called saturation effects (ref 2).

Recently, detailed experimental electrical transport studies of low resistivity amorphous alloys have been reported (ref 3). The present authors reported diffraction model studies (ref 4) of these alloys employing an effective t-matrix adjusted to satisfy the Friedel sum rule and to yield the observed magnitude of ρ. The surprising result of the theoretical analysis was that although qualitative agreement with the experimental results was obtained with the standard diffraction model, substantially improved quantitative agreement was obtained when saturation effects were incorporated into the model in a manner consistent with that employed to treat saturation effects in high resistivity metals (ref 5). That is, improved agreement with experiment was obtained when the Pippard-Ziman constraint (ref 6) on the electron-phonon interaction was included. (It had been shown previously that the Pippard-Ziman constraint can also provide a basis for understanding the electronic contribution to the ultrasonic attenuation (ref 6) at small $q\Lambda$, and the degradation of T_c in disordered superconductors (ref 7).)

References are listed at the end of this report.

The implications of the diffraction model incorporating phonon ineffectiveness through the Pippard-Ziman constraint for low resistivity alloys are explored in more detail in this report. A broader class of t-matrices as well as larger ranges of Λ and $2k_F/k_p$ than in Reference 4 are treated. We work in the context of the substitutional model (ref 8), which assumes the equality of all partial structure factors, but allows for different t-matrices for different species; thus, a better basis for interpretation of concentration dependent features of the T dependence of ρ than can be obtained in an effective potential treatment (ref 4) is established. We also restrict our analysis to binary alloys. The results specific to amorphous magnesium zinc (a-MgZn) alloys, for which $q_D\Lambda$ ranges between about 12 and 15 and $2k_F/k_p \approx 1.1$ are reported in Reference 9.

THEORETICAL MODELS

The diffraction model (ref 1) (Ziman-Faber theory) result for the electrical resistivity is

$$\rho = \frac{12\pi\Omega_o}{e^2 hV_F^2} \int_0^1 d[\frac{K}{2k_F}][\frac{K}{2k_F}]^3 |U(K)|^2 \tag{1}$$

where Ω_o is the atomic volume, V_F is the Fermi velocity, k_F is the Fermi wavevector, K is the scattering vector, h is Planck's constant divided by 2π, e is the electron charge, and in the "substitutional model," assuming a Debye phonon spectrum, and a binary alloy

$$|U(K)^2| = c_1c_2|t_1(K) - t_2(K)|^2 I^\rho(K) + |c_1t_1(K) + c_2t_2(K)|^2 S^\rho(K) \tag{2}$$

where c_i and $t_i(K)$ are the concentration and t-matrix for the i^{th} component,

$$S^{\rho}(K) = e^{-2W(K)}a(K) + \alpha \frac{\theta}{T} \left(\frac{K}{2k_F}\right)^2 \int_0^1 d\left(\frac{q}{q_D}\right)\left(\frac{q}{q_D}\right)^2 n(x)(n(x)+1)F(q\Lambda) \int \frac{d\Omega_q}{4\pi}\, a(\bar{K}+\bar{q}) \tag{3}$$

and

$$I^{\rho}(K) = e^{-2W(K)} + \alpha \frac{\theta}{T} \left(\frac{K}{2k_F}\right)^2 \int_0^1 d\left(\frac{q}{q_D}\right)\left(\frac{q}{q_D}\right)^2 n(x)[n(x)+1]F(q\Lambda) \tag{4}$$

in Sham-Ziman approximation. Here $e^{-2W(K)}$ is the Debye-Waller factor, $x = (\theta/T)(q/q_D)$, q_D the Debye wave number, θ the Debye temperature, T the temperature, $n(x) = (e^x-1)^{-1}$, $\alpha = 3(2\hbar k_F)^2/Mk_B\theta$, M is the averaged ionic mass, k_B is Boltzmann's constant. $F(q\Lambda)$ is referred to as the Pippard function and is given by

$$F(y) = \frac{2}{\pi}\left[\frac{y \tan^{-1} y}{y-\tan^{-1} y} - \frac{3}{y}\right] \tag{5}$$

We refer to $S^{\rho}(K)$ as the resistivity static structure factor. $I^{\rho}(K)$ is the resistivity static structure factor for a perfectly random array. $S^{\rho}(K)$ and $I^{\rho}(K)$ determine the temperature dependences of electrical transport quantities.

The geometric structure factors (assumed identical in the substitutional model) are given by

$$a(K) = a_{11}(K) = a_{22}(K) = a_{12}(K) = \frac{1}{N} \sum_{m,n} \exp[i\bar{K}\cdot(\bar{m}-\bar{n})] \tag{6}$$

where m and n run over averaged ionic positions. The scattering matrix elements (which incorporate single site multiple scattering) are given by

$$t_j(K) = \frac{2\pi\hbar^3}{m(2mE_F)^{1/2}\Omega_o} \sum(2\ell+1)\sin \eta_\ell^j(E_F)e^{i\eta_\ell^j(E_F)} P_\ell(\cos\theta) \tag{7}$$

where $\eta_\ell{}^j(E_F)$ is the scattering phase shift for angular momentum quantum number ℓ evaluated at the Fermi energy E_F for the j^{th} constituent, m is the electron mass, $P_\ell(x)$ is the ℓ^{th} Legendre polynomial and $\cos\theta = 1 - 2(K/2k_F)^2$. These equations are a generalization of those usually employed in studies of transport in liquid metals (ref 10) and will be discussed in more detail elsewhere.

We also give results based on the effective potential model. In this model, $t_1(K) \cong t_2(K) \cong t_E(K)$ and

$$|U_E(K)|^2 = S_E\rho(K)|t_E(K)|^2 \tag{8}$$

where $S_E{}^\rho(K)$ is defined analogously to $S^\rho(K)$ in Eq. (3) with the effective geometrical structure factor

$$a_E(K) = \sum_{ij} c_i c_j a_{ij}(K) \tag{9}$$

RESULTS

Results are given for an effective potential and for model t-matrices in a binary substitutional model. Percus-Yevick hard sphere structure factors (ref 11) (with packing fraction 0.525) are used to approximate a(K) and $a_E(K)$; the hard sphere diameters are varied to adjust $2k_F/k_p$ where k_p is the position of the principal structure factor peak.

The effective potential has phase shifts $\eta_\ell(E_F)$ given by 0.354, 0.294, -0.057, and 0.002 for $\ell = 0,1,2,3$, respectively, which yield approximate cancellation for $K \approx 1.6\ k_F$ and lead to ρ vs. T curves similar to those obtained in Reference 4 for Born approximation pseudopotentials in the large $q_D\Lambda$ limit. However, this effective potential heavily weighs backscattering and so is quite different in form from pseudopotentials. (These $\eta_\ell(E_F)$ were

computed for Zn with $X_\alpha = 0.85$.)

The t-matrices employed in the substitutional model calculations were computed using Herman and Skillman (ref 12) neutral atom wavefunctions for a-Mg_7Zn_3. The values of $\eta_\ell^j(E_F)$ are: −0.175, 0.085, 0.034, and 0.001 for Mg and 0.354, 0.294, −0.057, and 0.002 for Zn (as in the effective potential) for $\ell = 0$ to 3, respectively. (The phase shifts are quite sensitive to exchange. X_α was taken as 0.75 and 0.85 in Mg and Zn, respectively.) Very similar results (not discussed here) have been obtained for other t-matrices constructed to represent column I and column II metals in the substitutional model.

DISCUSSION OF RESULTS

The Temperature Coefficient of Resistivity (TCR)

Figure 1 shows graphs of tcr, the normalized TCR, where

$$\mathrm{tcr} \equiv (\theta/\alpha)\cdot\mathrm{TCR} = (\theta/\alpha\rho)d\rho/dT\big|_\theta$$

versus $2k_F/k_p$ for the two model potentials.

All the results were obtained with E_F fixed and $q_D = k_F$ which would not apply in an alloy series with varying electron-to-atom ratios. The curves were computed for $\alpha = 0.114$, but are very good approximations for reasonable values of α. One sees a shift of the region of negative TCR to larger values of $2k_F/k_p$ with respect to the results of the simple analysis based on the temperature dependence of the resistivity static structure factor by Meisel and Cote (ref 13). Futhermore, analysis of data in a-MgZn alloys indicates that 50 μΩcm corresponds to $q_D\Lambda$ near 12 which produces dramatic changes in the TCR from the predictions of standard ($q_D\Lambda = \infty$) Ziman-Faber theory.

Comparison of Figures 1(a) and 1(b) illustrates non-structural effects (i.e., effects produced by different scattering matrices) that might occur. One can also infer that (especially in cases for which $q_D\Lambda < 15$) the averaging required in treating real binary alloys - whose partial structure factor peaks might be separated by $k_p/10$ - would not yield qualitatively new effects; for example, about the same range of $2k_F/k_p$ would yield negative TCR.

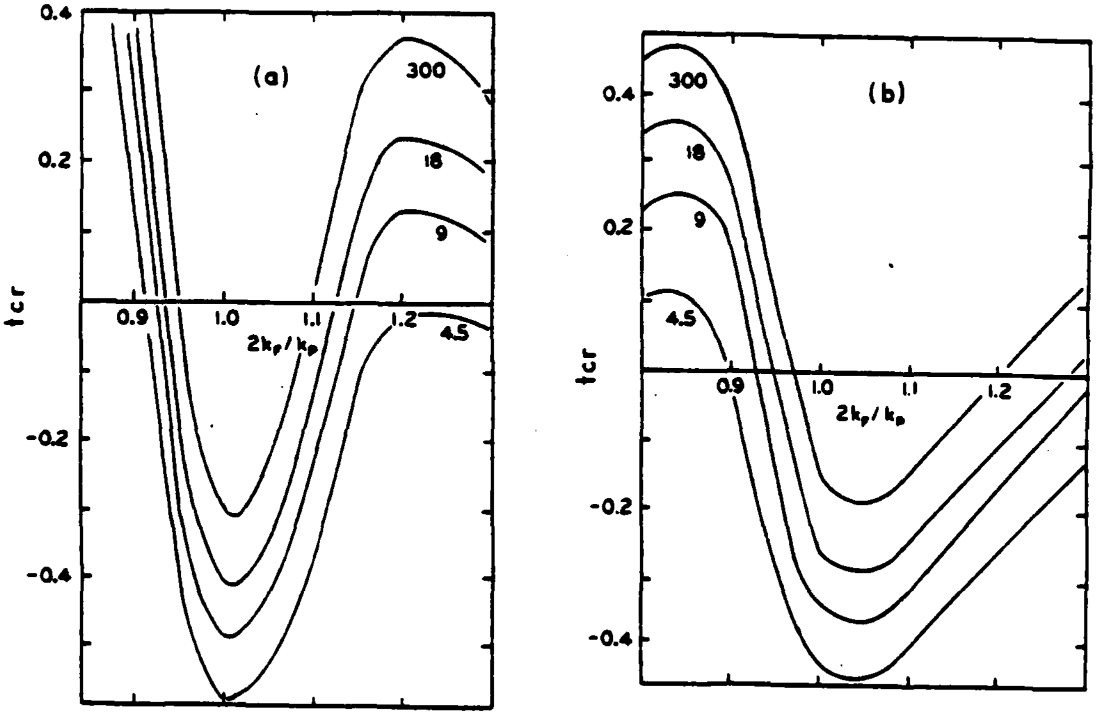

Figure 1. Normalized TCR vs. $2k_F/k_p$ for various $q_D\Lambda$. (a) For the effective potential. (b) For the substitutional model. $q_D\Lambda$ is indicated for each curve.

The Temperature Dependence of the Electrical Resistivity

Figure 2 shows results of calculations at various values of $2k_F/k_p$ and $q_D\Lambda$ for the substitutional model potential and also at $2k_F/k_p = 1.1$ for $q_D\Lambda = 8$ for the effective potential case. (Results at $2k_F/k_p = 1.11$ for the substitutional model applied to a-MgZn are shown in Reference 9. The graphs show the normalized relative change in the resistivity,

$$r \equiv (\rho(T) - \rho(\theta)/(\alpha\rho(\theta))$$

plotted against normalized temperature. (Most results were computed for $\alpha = 0.168$ but hold for reasonable α.)

The results show that deviations from standard diffraction model predictions can be explained by incorporating phonon ineffectiveness effects into the theory.

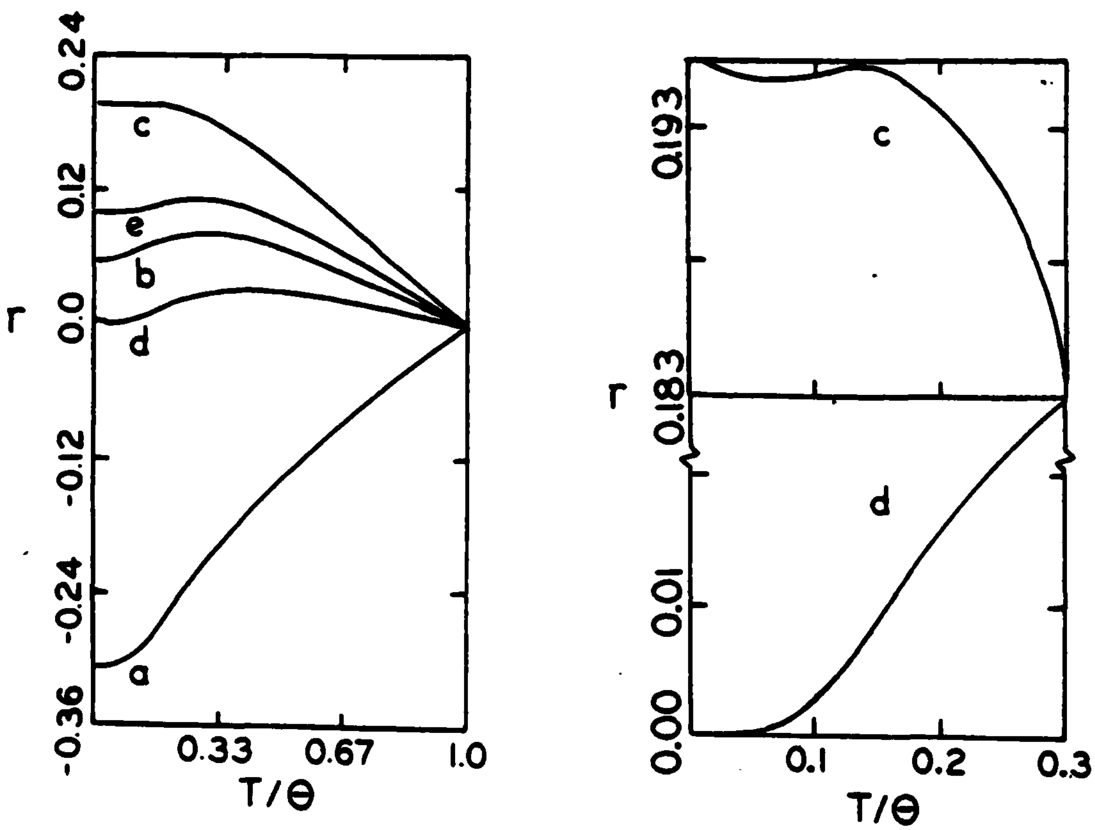

Figure 2. Normalized relative change in the resistivity vs. normalized temperature. Curves a-d are for the substitutional model. Curve e is for the effective potential. Details of curves c and d are shown below.

Curve	a	b	c	d	e
$2k_F/k_D$	0.9	1.0	1.0	1.2	1.1
$q_D\Lambda$	18	300	12	12	8

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